

# 3Alpha,6alpha-diphenylglycoluril

<b>Inchi:</b>	InChI=1S/C16H14N4O2/c21-13-17-15(11-7-3-1-4-8-11)16(19-13,20-14(22)18-15)12-9-5-
<b>InchiKey:</b>	WUDVGTHXCLJVJN-UHFFFAOYSA-N
<b>Formula:</b>	C16H14N4O2
<b>SMILES:</b>	O=C1NC2(c3ccccc3)NC(=O)NC2(c2ccccc2)N1
<b>Mol. weight [g/mol]:</b>	294.31
<b>CAS:</b>	5157-15-3

## Physical Properties

Property code	Value	Unit	Source
gf	500.64	kJ/mol	Joback Method
hf	139.09	kJ/mol	Joback Method
hfus	42.13	kJ/mol	Joback Method
hvap	89.16	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	1.318		Crippen Method
mcvol	210.120	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	971.18	K	Joback Method
tc	1291.58	K	Joback Method
tf	956.12	K	Joback Method
vc	0.771	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.87	J/molxK	971.18	Joback Method
cpg	720.56	J/molxK	1024.58	Joback Method
cpg	747.82	J/molxK	1077.98	Joback Method
cpg	777.20	J/molxK	1131.38	Joback Method
cpg	809.27	J/molxK	1184.78	Joback Method
cpg	844.58	J/molxK	1238.18	Joback Method
cpg	883.67	J/molxK	1291.58	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5157153&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5157153&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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